

Theory of non-local (pair site) reactivity from model static-density response functions

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Activation is a fundamental and well-known concept in chemistry. It may be qualitatively defined as an increase in the chemical reactivity pattern of a molecule at a given site k when the system is locally perturbed at a different site l , say. This external perturbation arise from a localized molecular rearrangement, a substitution, a selective solvation or simply by the approach of a reagent of variable hardness. This work presents a theoretical approach intending to quantify this activation concept in the density functional framework. This is done here by first calculating the fluctuation of the electron density at a given site k for the ground state of the isolated substrate (static reactivity model) and then incorporating the substrate and model electrophile reagents in a spatial disposition related to a virtual transition structure for the parent system. This perturbation is assumed representable by local changes in the external potential. It is shown that a local approximation to